

February 21, 2006

Mr. John Morris
American Chemistry Council
Aliphatic Esters Panel
1300 Wilson Boulevard
Arlington, VA 22209

Dear Mr. Morris:

The Office of Pollution Prevention and Toxics is transmitting EPA's comments on the robust summaries and test plan for Aliphatic Monoesters posted on the ChemRTK HPV Challenge Program Web site on February 19, 2004. I commend the Aliphatic Esters Panel for its commitment to the HPV Challenge Program.

EPA reviews test plans and robust summaries to determine whether the reported data and test plans will provide the data necessary to adequately characterize each SIDS endpoint. On its Challenge Web site, EPA has provided guidance for determining the adequacy of data and preparing test plans used to prioritize chemicals for further work.

EPA will post this letter and the enclosed comments on the HPV Challenge Web site within the next few days. As noted in the comments, we ask that the Panel advise the Agency, within 60 days of this posting on the Web site, of any modifications to its submission. Please send any electronic revisions or comments to the following e-mail addresses: oppt.ncic@epa.gov and chem.rtk@epa.gov.

If you have any questions about this response, please contact Mark Townsend, Chief of the HPV Chemicals Branch, at 202-564-8617. Submit questions about the HPV Challenge Program through the "Contact Us" link on the HPV Challenge Program Web site pages or through the TSCA Assistance Information Service (TSCA Hotline) at (202) 554-1404. The TSCA Hotline can also be reached by e-mail at tsca-hotline@epa.gov.

I thank you for your submission and look forward to your continued participation in the HPV Challenge Program.

Sincerely,

/s/

Oscar Hernandez, Director
Risk Assessment Division

Enclosure

cc: W. Penberthy
J. Willis

EPA Comments on Chemical RTK HPV Challenge Submission:

Aliphatic Monoesters Category

Summary of EPA Comments

The sponsor, the American Chemistry Council's Aliphatic Esters Panel, submitted a revised test plan and robust summaries for the Aliphatic Monoesters Category, dated November 26, 2003. EPA posted the submission on the ChemRTK HPV Challenge Website on February 19, 2004. The category consists of Palmitic acid, 2-ethylhexyl ester (CAS No. 29806-73-3), Stearic acid, tridecyl ester (CAS No. 31556-45-3) and tall oil fatty acids, 2-ethylhexyl esters (CAS. No. 68334-13-4). Robust summaries for six structural analogs were also submitted.

EPA has reviewed this submission and has reached the following conclusions:

1. Category Definition. The category is clearly defined.
2. Category/Analog Justification. The submitter's support for grouping the chemicals under this category and for the use of the proposed analogs is adequate.
3. Physicochemical Properties. The submitter needs to provide measured melting point and vapor pressure data for the three chemicals in this category.
4. Environmental Fate. Although the submitted data are adequate for these endpoints for the purposes of the HPV Challenge Program, the submitter needs to provide robust summaries for photodegradation, stability in water, and fugacity.
5. Health Effects. Adequate data were submitted for all endpoints except chromosomal aberrations. EPA agrees that the submitter's technical discussion for chromosomal aberrations addresses the endpoint for the purposes of the HPV Challenge Program.
6. Ecological Effects. Although no data are available for category chemicals and the available data for fish, daphnia, and algae on an analog monoester are inadequate, EPA considers no additional testing is warranted because of low water solubility and high log Kow for the members of this category.

EPA requests that the submitter advise the Agency within 60 days of any modifications to its submission.

EPA Comments on the Aliphatic Monoesters Category Challenge Submission

Category Definition

The submission covers two discrete chemicals, the 2-ethylhexyl ester of palmitic acid and tridecyl ester of stearic acid and one mixture, 2-ethylhexyl esters of tall oil fatty acids. The esters range in carbon number from C24 to C31. The submitter also included six other aliphatic monoesters as analogs for the category members. The analogs range in carbon number from C22 to C34: butyl stearate (CAS No. 123-95-5); 2-ethylhexyl esters of C16-18 saturated and C18 unsaturated fatty acids (CAS No. 85049-37-2); octyl stearate, (CAS No. 109-36-4); decyl oleate (CAS No. 3687-46-5); tridecyl stearate (CAS No. 31556-45-3); myristyl stearate (CAS No. 17661-50-6); and isocetyl stearate (CAS No. 25339-09-7). The sponsor proposes using test data from these substances to characterize the three sponsored substances.

The submitter states that the chemical 2-ethylhexyl esters of tall oil fatty acids is composed mainly of 2-ethylhexyl esters of oleic and linoleic acid but does not give a more detailed composition of the mixture. It is known that fatty acids obtained from the distillation of tall oils may contain other fatty acids (i.e., C16 fatty acids) and resin acids. A more detailed description of the substance is needed in order to verify that the 2-ethylhexyl esters of oleic and linoleic acid are the predominant components.

Category and Analogs Justification

The submitter's rationale for grouping the sponsored and analog substances is based on the chemical and structural similarities which are expected to result in similar physicochemical, environmental fate, and toxicological properties. The structures of the category members and the analogs are close and their grouping into a single category is supported. However, it should be noted that only one of the analogs is a 2-ethylhexyl ester whereas two of the three sponsored chemicals have this group.

Test Plan

Physicochemical Properties (melting point, boiling point, vapor pressure, partition coefficient, water solubility)

The data provided by the submitter for boiling point, partition coefficient, and water solubility are adequate for the purposes of the HPV Challenge Program.

Melting point. The submitted estimated data are not adequate for the purposes of the HPV Challenge Program. For example, the EPIWIN-estimated melting point for stearic acid, tridecyl ester (190 °C) is far higher than the reported value of 49.2–49.6 °C (Beilstein On-line Search, June 20, 2005) which underlines the known large error tendency in calculating this endpoint. The submitter needs to provide measured melting point data for the three category chemicals.

Vapor pressure. The submitted estimated data provided in Table 2 of the test plan for palmitic acid, 2-ethylhexyl ester and tall oil fatty acids, 2-ethylhexyl ester are not adequate for the purposes of the HPV Challenge program because they are above the 1×10^{-5} Pa testing threshold for this endpoint. The submitter needs to provide measured vapor pressure data for these two substances. The submitter's value for stearic acid, tridecyl ester barely exceeds the threshold value and can be considered adequate.

Environmental Fate (photodegradation, stability in water, biodegradation, fugacity)

Although the submitted data, as described in Table 2 of the test plan, for all SIDS endpoints are adequate for the purposes of the HPV Challenge Program, the submitter needs to provide robust summaries for photodegradation, stability in water, and fugacity.

Stability in water. In Table 2 of the test plan there is an error for tall oil fatty acids, 2-ethylhexyl ester where the submitter gives a half-life of 0.0561/mol-second, which EPA assumes is the calculated rate constant. The submitter needs to make the appropriate correction.

Health Effects (acute toxicity, repeated-dose toxicity, genetic toxicity, and reproductive/developmental toxicity)

Only acute toxicity data have been submitted for two of the three sponsored category members (2-ethylhexyl ester of palmitic acid and 2-ethylhexyl esters of tall oil fatty acids) with minimum details; no human health data were submitted for the tridecyl ester of stearic acid. However, from the available data on the sponsored substances and the consistently low toxicity demonstrated by the available data on analogs EPA agrees that no new information would be gained from further animal testing for the purposes of the HPV Challenge Program.

Acute toxicity. Although acute toxicity data were submitted for all analogs, the submitter provided a reliability rating of 4 ("unassignable") in five of the six analogs' robust summaries because the data were from the European Chemical Bureau's IUCLID data sets. EPA considers this endpoint has been addressed for the purposes of the HPV Challenge Program because of the available data for the sponsored substances and minimal supporting information on the analogs.

Genetic toxicity (chromosomal aberrations). The submitter did not provide data for this endpoint or propose testing. A technical discussion on the likelihood that this class of compounds exhibits no clastogenic behavior was provided along with supporting data on long-chain carboxylic acid esters. This discussion adequately addresses this endpoint for the purposes of the HPV Challenge Program.

Ecological Effects (fish, invertebrates, and algae)

No aquatic toxicity data are available on the category chemicals. The submitted aquatic toxicity data on an analog, 2-ethylhexyl esters of C16-18 saturated and C18 unsaturated fatty acids, are inadequate because all studies were conducted above the chemical's water solubility limit and thus are inadequate for read-across purposes (the robust summaries also lack critical details). However, EPA agrees with the submitter that additional testing is not warranted given the low water solubility (calculated <1ppb) and high log Kow (>9) of the members of this category.

Specific Comments on the Robust Summaries

No comments.

Followup Activity

EPA requests that the submitter advise the Agency within 60 days of any modifications to its submission.